Appl. No. 10/669,705
Hao Chen et al.
Reply to Office Action of July 6, 2006

Amendments to the Claims:

This listing of claims will replace all prior versions, and listings, of claims in the application:

Listing of Claims:

1. (Currently amended) A method of drug discovery and development comprising:

providing a full-rank database of interactions between a plurality of molecular targets and a plurality of compounds, wherein the database comprises a set of descriptors that describe structural features of the molecular targets and the compounds;

selecting ~~using one or more databases comprising chemical and biological interaction data and one or more computer-based data analysis programs to identify compounds that have desired activity at~~ two or more molecular targets that are associated with a disease state for which the drug discovery and development are directed;

analyzing the database to identify a set of compound descriptors associated with a set of desired interactions with the two or more molecular targets;

selecting a plurality of candidate compounds as potential drugs to treat the disease state;

representing each of the candidate compounds in terms of the descriptors; and

identifying the candidate compounds with the set of compound descriptors associated with the set of desired interactions.

2. (Currently amended) The method of claim 1, wherein the ~~drug discovery and development are directed to identifying additional applications and uses of~~plurality of candidate compounds comprise known compounds.

3. (Currently amended) The method of claim 1, wherein the ~~drug discovery and development are directed to identifying multiple targets relevant to the treatment of a specific disease state~~analyzing step comprises reverse partitioning.

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4. (Currently amended) The method of claim 1, wherein the ~~drug discovery and development are directed to *in silico* identification of compounds that display patterns of activity at two or more molecular targets that are associated with a disease state~~descriptors comprise 2-D bond length descriptors.

5. (Currently amended) A method of drug discovery and development comprising:

providing a full-rank database of interactions between a plurality of molecular targets and a plurality of compounds, wherein the database comprises a set of descriptors that describe structural features of the molecular targets and the compounds;

analyzing the database to identify a set of compound descriptors associated with both ~~using one or more databases comprising chemical and biological interaction data and one or more computer-based data analysis programs to identify compounds that~~ (a) have a desired activity at one or more molecular targets that are associated with a disease state for which the drug discovery and development are directed and (b) ~~do not have~~ an undesired activity ~~or have substantially reduced activity that is undesired~~ at one or more molecular targets that are associated with ~~possible side~~undesired therapeutic effects; ~~toxicity; adverse absorption, distribution, metabolism, or elimination (ADME) properties; or other properties not intended to be manifested by compounds being developed to treat the disease state associated with the drug discovery~~

representing a drug candidate in terms of the descriptors; and

determining whether the compound contains the set of compound descriptors.

6. (Currently amended) The method of claim 5, wherein the drug ~~discovery and development are directed to identifying additional applications and uses of~~candidate is a known compounds.

7. (Currently amended) The method of claim 5, wherein the ~~drug discovery and development are directed to identifying~~there are multiple targets ~~relevant to the treatment of~~ a~~a~~ssociated with the ~~specific~~ disease state.

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8. The method of claim 5, wherein the ~~drug discovery and development efforts are directed to *in silico* identification of compounds that display patterns of activity and inactivity at two or more molecular targets that are associated with a disease state~~undesired therapeutic effect is a side effect.

9 - 37. (Canceled)

38. (New) The method of claim 5, wherein the undesired therapeutic effect is toxicity.

39. (New) The method of claim 5, wherein the undesired therapeutic effect is related to adsorption, distribution, metabolism, or elimination.

40. (New) The method of claim 5, wherein the descriptors comprise 2-D bond length descriptors.

41. (New) The method of claim 5, wherein the analyzing step comprises reverse parititioning.